

Modern Physics Letters B
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Classical thermodynamics from quasi-probabilities

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Received (Day Month Year)

Revised (Day Month Year)

The basic idea of a microscopic understanding of Thermodynamics is to derive its main features from a microscopic probability distribution. In such a vein, we investigate the thermal statistics of quasi-probabilities's semi-classical analogs in phase space for the important case of quadratic Hamiltonians, focusing attention in the three more important instances, i.e., those of Wigner, P -, and Husimi distributions. Introduction of an effective temperature permits one to obtain a unified thermodynamic description that encompasses and unifies the three different quasi-probability distributions. This unified description turns out to be classical.

Keywords: Semiclassical physics; P -function; Information quantifiers; thermal properties

1. Introduction

A quasi-probability (QP) distribution is a mathematical construction resembling a probability distribution. It does not necessarily fulfill, though, some of the Kolmogorov axioms for probabilities¹. QPs display general features of ordinary probabilities and yield expectation values with respect to the weights of the distribution. However, they disobey the third probability postulate¹, in the sense that regions integrated under them do not represent probabilities of mutually exclusive states. Some quasi-probability distributions exhibit zones of negative probability density.

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QPs often arise in trying to study quantum mechanics a phase space representation. This is frequently done in quantum optics, time-frequency analysis, etc.

The dynamics of a quantum system is determined by a master equation. We speak of an equation of motion for the density operator ($\hat{\rho}$), defined with respect to a complete orthonormal basis. One can show that the density can always be written in a diagonal manner, with respect to an overcomplete basis ². If this basis is that of coherent states $|\alpha\rangle$ one has ^{2,3}

$$\hat{\rho} = \int \frac{d^2\alpha}{\pi} P(\alpha, \alpha^*) |\alpha\rangle\langle\alpha|, \quad (1)$$

where $d^2\alpha/\pi = dx dp/2\pi\hbar$, with x and p variables of the phase space. The system evolves as prescribed by the evolution of the quasi-probability distribution function. Coherent states, eigenstates of the annihilation operator \hat{a} , serve as the overcomplete basis in such a build-up ^{2,3}.

There exists a family of different representations, each connected to a different ordering of the creation and destruction operators \hat{a} and \hat{a}^\dagger . Historically, the first of these is the Wigner quasi-probability distribution W ⁴, related to symmetric operator ordering. In quantum optics the particle number operator is naturally expressed in normal order and, in the pertinent scenario, the associated representation of the phase space distribution is the Glauber–Sudarshan P one ³. In addition to W and P , one may find many other quasi-probability distributions emerging in alternative representations of the phase space distribution ⁵. A quite popular representation is the Husimi Q one ^{6,7,8,9}, used when operators are cast in anti-normal order.

In this paper we wish to apply *semiclassical information theory tools* associated to these P , Q , and W representations (for quadratic Hamiltonians) *in order to describe the concomitant thermal semiclassical features*. We specialize things to the three f -functions associated to a Harmonic Oscillator (HO) of angular frequency ω . In such a scenario the three functions –that we name for sake of convenience f_P , f_Q , and f_W – are simple Gaussians and the treatment becomes entirely analytical, a very convenient feature. The HO is a really important system that yields insights usually having a wide impact. Thus, the HO constitutes much more than a mere simple example. Nowadays, it is of particular interest for the dynamics of bosonic or fermionic atoms contained in magnetic traps ^{10,11,12} as well as for any system that exhibits an equidistant level spacing in the vicinity of the ground state, like nuclei or Luttinger liquids.

In this paper we are interested in thermal states regarded as semi-classical distributions in phase space –analogs of the quantum quasi-probabilistic distributions. We will try to ascertain what physical Thermodynamics’ features are they able to describe at the semi-classical level. These distributions are ^{13,14}

$$f_P = \gamma_P e^{-\gamma_P |\alpha|^2}, \quad \gamma_P = e^{\beta\hbar\omega} - 1 \quad (P - \text{function}), \quad (2)$$

$$f_Q = \gamma_Q e^{-\gamma_Q |\alpha|^2}, \quad \gamma_Q = 1 - e^{-\beta \hbar \omega} \quad (Q - \text{function}), \quad (3)$$

$$f_W = \gamma_W e^{-\gamma_W |\alpha|^2}, \quad \gamma_W = 2 \tanh(\beta \hbar \omega / 2) \quad (W - \text{function}), \quad (4)$$

with $\beta = 1/k_B T$, k_B the Boltzmann constant, and T the temperature. As stated above, these distributions will be used in the next section as semiclassical statistical weight functions. Since ours is NOT a quantum approach, the ordering of the HO-creation and destruction operators a and a^\dagger plays no role whatsoever in our manipulations below.

This paper is organized as follows: section 2 refers to information quantifiers, in a phase space representation, for Gaussian distributions. In Section 3 we focus attention upon thermodynamic relations and we express them in terms of an effective temperature. Finally, some conclusions are drawn in Section 4.

2. Semi-classical information quantifiers

- The first step in our development is to calculate entropic quantifiers for these Gaussian distributions. In order to simplify the notation we will consider a general normalized gaussian distribution in phase space

$$f(\alpha) = \gamma e^{-\gamma |\alpha|^2}, \quad (5)$$

whose normalized variance is $1/\gamma$ and γ taking values γ_P , γ_Q and γ_W given by Eqs. (2), (3), and (4), respectively.

The logarithmic Boltzmann's information measure for the the probability distribution (5) is

$$S = - \int \frac{d^2 \alpha}{\pi} f(\alpha) \ln f(\alpha) = 1 - \ln \gamma, \quad (6)$$

so that it acquires the particular values

$$S_P = 1 - \ln(e^{\beta \hbar \omega} - 1), \quad (7)$$

$$S_Q = 1 - \ln(1 - e^{-\beta \hbar \omega}), \quad (8)$$

$$S_W = 1 - \ln(2 \tanh(\beta \hbar \omega / 2)), \quad (9)$$

for, respectively, the distributions f_P , f_Q , and f_W .

- Next, we focus attention on the information quantifier known as Fisher's information measure. We specialize it for families of shift-invariant distributions, that do not change shape under translations. One has^{15,16}

$$I = \int dx f(x) \left(\frac{\partial \ln f(x)}{\partial x} \right)^2, \quad (10)$$

and, in phase space, it adopts the appearance¹⁷

$$I = \frac{1}{4} \int \frac{d^2\alpha}{\pi} f(\alpha) \left(\frac{\partial \ln f(\alpha)}{\partial |\alpha|} \right)^2, \quad (11)$$

such that considering $f(\alpha)$ given by Eq. (5) we get $I = \gamma$, whose specific values are $\gamma_P, \gamma_Q, \gamma_W$ for the three functions f_P, f_Q , and f_W , respectively.

- The statistical complexity is a functional $C[P]$ that can primarily be viewed as a quantity that characterizes the probability distribution P . It quantifies not only randomness but also the presence of correlational structures¹⁸. The opposite extremes of perfect order and maximal randomness possess no structure to speak of. In between these two special instances, a wide range of possible degrees of physical structure exist, degrees that should be reflected in the features of the underlying probability distribution. The statistical complexity C , according to López-Ruiz, Mancini, and Calvet¹⁸, is a suitable product of two quantifiers, such that C becomes minimal at the extreme situations of perfect order or total randomness. Instead of using the prescription of¹⁸, but without violating its spirit, we will take one of these two quantifiers to be Fisher's measure and the other an entropic form, since it is well known that the two behave in opposite manner¹⁹. Thus:

$$C = SI = \gamma (1 - \ln \gamma), \quad (12)$$

that vanishes for perfect order or total randomness. For each particular case, we explicitly have

$$C_P = (e^{\beta\hbar\omega} - 1) [1 - \ln(e^{\beta\hbar\omega} - 1)], \quad (13)$$

$$C_Q = (1 - e^{-\beta\hbar\omega}) [1 - \ln(1 - e^{-\beta\hbar\omega})], \quad (14)$$

$$C_W = (2 \tanh(\beta\hbar\omega/2)) [1 - \ln(2 \tanh(\beta\hbar\omega/2))], \quad (15)$$

for, respectively, the distributions f_P, f_Q , and f_W . The maximum of the statistical complexity occurs when $\gamma = 1$ and, the associated temperature values are

$$\begin{cases} e^{\beta\hbar\omega} - 1 = 1 \Rightarrow T = \hbar\omega/k_B \ln 2 & \text{for the } f_P\text{-function,} \\ 1 - e^{-\beta\hbar\omega} = 1 \Rightarrow T = 0 & \text{for the } f_Q\text{-function,} \\ 2 \tanh(\beta\hbar\omega/2) = 1 \Rightarrow T = \hbar\omega/2k_B \arctan(1/2) & \text{for the } f_W\text{-function.} \end{cases}$$

3. Thermodynamic relations

We start this section considering the semi-classical Hamiltonian of the harmonic oscillator that reads

$$\mathcal{H}(x, p) = \hbar\omega|\alpha|^2 = \hbar\omega \left(\frac{x^2}{4\sigma_x^2} + \frac{p^2}{\sigma_p^2} \right), \quad (17)$$

where x and p are phase space variables and $\sigma_x^2 = \hbar/2m\omega$ and $\sigma_p^2 = \hbar m\omega/2$ ²⁰. Let us further define the semiclassical expectation value of the function $\mathcal{A}(x, p)$ as

$$\langle \mathcal{A} \rangle_f = \int \frac{d^2\alpha}{\pi} f(\alpha) \mathcal{A}(x, p), \quad (18)$$

indicating that $f(\alpha)$ is the statistical weight function. Thus, the mean energy of the hamiltonian $\mathcal{H}(x, p)$ is written in the fashion

$$U^* = \hbar\omega \int \frac{d^2\alpha}{\pi} f(\alpha) |\alpha|^2 = \frac{\hbar\omega}{\gamma}, \quad (19)$$

where γ takes the respective values γ_P , γ_Q , and γ_W explained in Introduction. Additionally, the thermodynamic entropy S' is

$$S' = k_B(1 - \ln \gamma), \quad (20)$$

where we have added the Boltzmann constant k_B . The mean energy can be viewed as a function of the thermodynamic entropy S' , in the following fashion. Combining (19) with the thermodynamic entropy (20) we get the associated, fundamental equation $U^* = U^*(S')$

$$U^*(S') = \hbar\omega e^{S'/k_B - 1}, \quad (21)$$

and

$$\gamma = e^{1 - S'/k_B}. \quad (22)$$

Thus, the differential of U^* becomes

$$dU^* = \left(\frac{\partial U^*}{\partial S'} \right)_V dS', \quad (23)$$

where we have considered the volume V to be constant. Thus, after effecting the pertinent replacements we find

$$dU^* = \frac{\hbar\omega}{k_B\gamma} dS', \quad (24)$$

which suggests introducing an effective temperature T_{eff} . *Using T_{eff} we obtain a unified picture that encompasses the three distributions f_P , f_Q , and f_W , in a single thermodynamic description.* We have

$$T_{eff} = \left(\frac{\partial U^*}{\partial S'} \right)_V = \frac{\hbar\omega}{k_B\gamma}, \quad (25)$$

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such that

$$dU^* = T_{eff} dS'. \quad (26)$$

Note that in the three instances, $T_{eff} = \infty$ for $T = \infty$. However, if $T = 0$, $T_{eff} = 0$ only in the f_P -case. It equals $1/2$ in the Wigner instance and equals 1 in the Husimi case, as depicted in the accompanying figure.

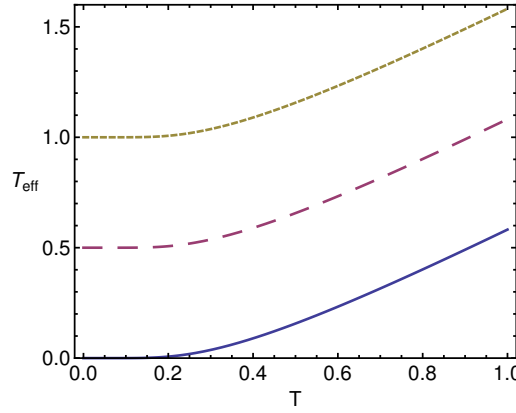


Fig. 1. Effective temperature T_{eff} versus temperature T in $(\hbar\omega/k_B)$ -units.

From (19) and (26) we can rewrite the mean energy in terms of effective temperature.

$$U^* = k_B T_{eff}, \quad (27)$$

that corresponds to the classical mean energy of a harmonic oscillator of temperature T_{eff} , with $k_B T_{eff}/2$ contributions for each of the two pertinent degrees of freedom. Similarly, the thermodynamic entropy is recast as

$$\frac{S'}{k_B} = 1 + \ln \left(\frac{k_B T_{eff}}{\hbar\omega} \right), \quad (28)$$

and the Helmholtz free energy is given by

$$A^* = U^* - T_{eff} S' = k_B T_{eff} \ln \left(\frac{\hbar\omega}{k_B T_{eff}} \right). \quad (29)$$

The effective specific heat is defined as

$$C_V^* = \left(\frac{\partial U^*}{\partial T_{eff}} \right)_V, \quad (30)$$

that using (27) becomes

$$C_V^* = k_B, \quad (31)$$

which is precisely the specific heat for the classical harmonic oscillator which is independent of the temperature. This becomes the Dulong and Petit's rule at the classical limit. In view of (26) and (29) the analog partition function Z^* is given by

$$Z^* = \frac{1}{\gamma}, \quad (32)$$

and, according to Eqs. (6), (19), and (32) we find

$$S' = \ln Z^* + \beta^* U^*, \quad (33)$$

with

$$\beta^* = \frac{1}{k_B T_{eff}} = \frac{\gamma}{\hbar\omega}. \quad (34)$$

Thus, one reobtains all the thermal results pertaining to a classical HO at the temperature T_{eff} . Note that the whole thermal description becomes now of a classical character. All the quantum effects pertaining to the probability distributions are contained in the relationship (24) between T_{eff} and T .

It is interesting to look at the statistical complexity C in order to see at what effective temperature the possible correlational structures carried by our probabilistic distributions are stronger. Expressed in terms of T_{eff} , C becomes

$$C' = IS' = \frac{\hbar\omega}{T_{eff}} \left[1 + \ln \left(\frac{k_B T_{eff}}{\hbar\omega} \right) \right]. \quad (35)$$

Keeping in mind T_{eff} 's definition, it is easy to see that the maximum for the complexity C' is attained when $T_{eff} = \hbar\omega/k_B$. This implies, according to Eq. (25) that the maximum of the Fisher measure is $I_{max} = 1$. At the complexity-peak, thermodynamic quantities take the values

$$U_{max}^* = \hbar\omega, \quad (36)$$

$$S'_{max} = k_B, \quad (37)$$

$$C'_{max} = k_B, \quad (38)$$

a remarkable simplicity!

4. Conclusions

We have investigated here the thermal statistics of quasi-probabilities-analogs $f(\alpha)$ in phase space for the important case of quadratic Hamiltonians, focusing attention on the three more important instances, i.e., those of Wigner, P -, and Husimi distributions.

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- Introduction of an effective temperature permits one to obtain a unified thermodynamic description that encompasses the three different quasi-probability distributions. This unified description turns out to be classical.
- The above entails that all possible “quasi-quantum” effects have to be contained in the relationship between T_{eff} and T . Note, for instance, that the minimal energy is not zero (*one of these effects*) but, in the f_W -case, $T_{eff}^W = \hbar\omega/2k_B$, implying a minimum energy $k_B T_{eff}^W = \hbar\omega/2$. Additionally, the Husimi- $T_{eff}^Q = \hbar\omega/k_B$ reflects the well known fact that the Husimi distribution “smoothes” the Wigner one over a phase-space area $= \hbar$.
- The basic idea of a microscopic understanding of thermodynamics is to derive its main features from a microscopic probability distribution. We have done just this using as distributions quasi-probability ones.

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